CLAIMS

What Is Claimed Is:

1. A method comprising:

predicting a secondary structure of a protein;

superimposing the predicted secondary structure on a set of topomers;

refining the superimposed secondary structure; and

predicting a tertiary structure of a protein

2. The method of claim 1, wherein said secondary structure is a consensus secondary structure prediction.

3. The method of claim 1, further comprising annealing the secondary structure by energy minimization.

4. The method of claim 3, wherein said energy minimization is by a random Monte Carlo method.

5. The method of claim 4, wherein the random Monte Carlo method uses random moves from a log probability table.

6. The method of claim 3, wherein the random Monte Carlo method uses smart moves.

7. The method of claim 1, wherein the secondary structure superimposed on a set of topomers is refined by energy minimization.

8. The method of claim 7, wherein the secondary structure superimposed on a set of topomers is refined using a molecular modeling program.

9. The method of claim 8, wherein the molecular modeling program is X-PLOR.

10. A method comprising:

predicting a secondary structure of a protein;

generating a three-dimensional representation of the predicted secondary structure;

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4   optimizing the secondary structure by adjusting dihedral angles using smart moves; and

5   determining a three-dimensional protein structure by modeling the optimized secondary

6   structure on a topomer model.

1   11.   The method of claim 10, wherein said secondary structure is a consensus

2   secondary structure prediction.

1   12.   The method of claim 10, wherein optimization is performed using a random

2   Monte Carlo method.

1   13.   The method of claim 12, wherein the random Monte Carlo method is used in

2   conjunction with a localized energy function.

1   14.   The method of claim 10, wherein said three-dimensional structure model is

2   refined using simulated annealing.

1   15.   A machine readable medium that provides instructions, which when executed

2   by a machine cause said machine to perform a method comprising:

3   predicting a secondary structure of protein;

4   superimposing the secondary structure on a topomer model; and

5   refining the topomer model.

1   16.   A machine readable medium as in claim 15, wherein said secondary structure is

2   a consensus secondary structure prediction.

1   17.   A machine readable medium as in claim 15, further comprising energy

2   minimization of the secondary structure prediction.

1   18.   A machine readable medium as in claim 17, wherein said energy minimization

2   is by a random Monte Carlo method.

1   19.   A machine readable medium as in claim 18, wherein random moves are selected

2   from a log probability table.

1   20.   A machine readable medium as in claim 15, wherein the topomer model is
2   refined by topological entropy minimization.

1   21.   A machine readable medium as in claim 20, wherein the topomer model is
2   refined by a molecular modeling program.